Improved Interface Treatment in Arbitrary Lagrangian-Eulerian Simulations using the Moment-of-Fluid Method

M. Kucharik, FNSPE, Czech Technical University in Prague; Rao V. Garimella, Samuel P. Schofield, Mikhail J. Shashkov, T-5

We have successfully extended the Moment-of-fluid (MOF) interface reconstruction and tracking method to Arbitrary Lagrangian-Eulerian (ALE) compressible, multimaterial, multiple equation-of-state hydrodynamic simulations. In these simulations, the MOF method shows significant improvement over existing interface reconstruction methods.

In Lagrangian hydrodynamic simulations the equations of conservation of mass, momentum, and energy are solved in a Lagrangian reference frame where the computational mesh moves with the material. However, for many flows, vorticity or shear in the flow may ultimately tangle the mesh and terminate the simulation. This has led to the development of ALE methods where the mesh may move with a different velocity than the computed flow field in order to preserve mesh quality.

ALE simulations consist of three steps: 1) a Lagrangian phase, where the equations are solved in the Lagrangian reference frame, 2) a mesh smoothing phase, where a better quality mesh is determined based on the initial mesh or the mesh at the end of the Lagrangian step (this step may be done after a set number of Lagrangian steps or when a mesh quality threshold is reached), and 3) a remap phase, where conserved variables are interpolated from the Lagrangian mesh of step 1 to the smoothed mesh from step 2 in a conservative manner.

In a pure Lagrangian calculation material interfaces are preserved through the calculation assuming they are originally at cell boundaries. However, for ALE simulations interfaces will no longer be aligned with the mesh and an interface treatment is necessary. ALE simulations have traditionally tracked the fractional volumes and used interface reconstruction [1] to approximate the interface positions in each mesh cell when required. In the interface reconstruction process, a line segment representing the interface within the cell is positioned to match the prescribed material volume. Interface reconstruction methods are primarily differentiated by how the orientation of the line is determined. The widely used first-order-accurate Youngs method [2] uses the negative gradient of the volume fractions as the outward normal. It works well for two materials but has an artificial material order dependency when reconstructing interfaces for more than two materials. The MOF method [3], developed at LANL, utilizes the first moments in addition to fractional volumes of the materials to reconstruct the interface. It is material-order independent and can correctly locate each material in a cell providing true sub-cell resolution.

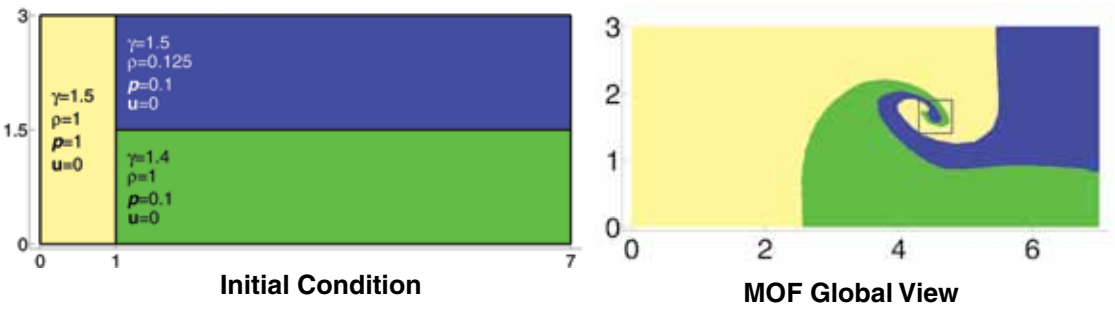
However, in compressible flow simulations the fractional volumes are not necessarily a Lagrangian invariant and the time evolution of the first moments must account for the volumetric change. This has impeded the adoption of MOF in compressible and ALE simulations, although MOF has shown significant improvements in incompressible flow simulations [4].

In this work, we have developed a method to update the centroid in the Lagrangian phase that is provably second-order accurate, and we have developed a method to update the material moments in the remap phase that preserves the accuracy of the MOF method.

To update material centroids during the Lagrangian phase, the material centroid in a cell is assumed to be constant in barycentric coordinates before and after the Lagrangian step. We have shown [5] this provides a second-order accurate approximation to the true evolution of a material centroid. This approach is very general, working for arbitrary convex polygonal mesh cells.

During the remap step, the material moments on the new, smoothed mesh are calculated using an intersection-based remap written in flux form to provide conservation to machine accuracy. The overall method has been shown to be robust and accurate.

In the triple-point problem, a high-pressure region in the left of the 7× 3 domain expands into two layers of different gases as shown in Fig. 1. Here ρ is the density, p is the pressure, **u** is the velocity and γ is the adiabatic exponent. The top, blue material compresses more readily, allowing the shock wave to travel faster than in the bottom green material. As a result, strong rotation is generated at the interface between the three materials. This vortex creates problems for the Lagrangian simulation, but the ALE simulation handles it gracefully – but it must reconstruct the interfaces.



Because Youngs method is material-order dependent, that is, the reconstructed interfaces depend on the order they were processed, different material orderings may give different results. This is shown in the zoomed-in portion of Fig. 1 where different orderings have caused mixing or separation of the material interfaces. MOF not only accurately preserves the interfaces, it can evaluate all possible material orderings and choose the optimal configuration locally.

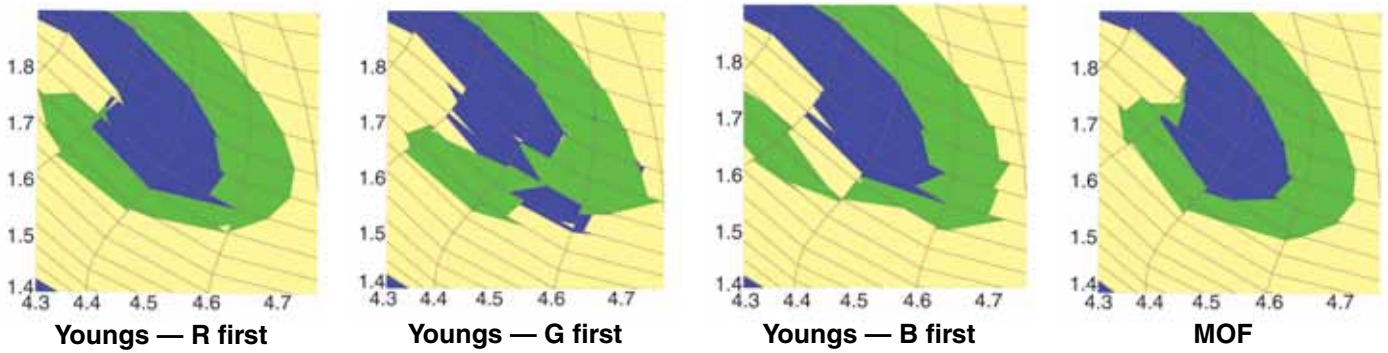


Fig. 1. The initial condition and material positions for the triple-point problem at time T =5.0. The mesh was relaxed using the Winslow method [6] after every 20 Lagrangian steps. The zoomed-in portion shows the material positions with different material orderings and with the MOF method. The mesh consists of 140 × 60 cells with material interfaces initially aligned with the mesh.

For more information contact Samuel P. Schofield at sams@lanl.gov.

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